

Electronic Supplementary Information (ESI)

# **The nature of stability and adsorption interactions of binary Au-Li clusters with bridge adsorption structures**

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(1) The cartesian coordinates of (AuLi)<sub>n</sub> (n = 1-9) clusters

n = 1

Au	0.000000	-0.000000	0.083272
Li	-0.000000	0.000000	-2.192832

n = 2

Au	2.053730	0.000000	-0.000001
Au	-2.053732	-0.000001	-0.000001
Li	0.000000	1.355106	0.000027
Li	0.000039	-1.355089	0.000027

n = 3

Au	1.095869	1.891130	0.000005
Au	-2.283798	-0.003624	-0.000000
Au	1.102525	-1.887635	-0.000005
Li	2.640686	0.004457	-0.000049
Li	-0.195800	-0.000734	1.304317
Li	-0.195905	-0.000341	-1.304266

n = 4

Au	-2.413129	0.252584	-0.568192
Au	1.050484	2.250541	0.183802
Au	0.219963	-1.198298	2.171445
Au	1.142666	-1.304830	-1.787056
Li	-0.776741	-1.665168	-0.137074
Li	-0.845115	0.965895	1.321776
Li	1.785815	-0.187053	0.421331
Li	-0.163539	0.886376	-1.606028

n = 5

Au	1.878229	-1.923295	-0.623716
Au	1.923991	1.877529	-0.623706
Au	0.000138	-0.000119	2.393049
Au	-1.924136	-1.877572	-0.623683
Au	-1.878220	1.923457	-0.623517
Li	-0.027080	-2.241188	0.933572
Li	2.241448	-0.026998	0.934605
Li	-0.000139	-0.000157	-1.061755
Li	0.027113	2.241269	0.933687
Li	-2.241404	0.027062	0.934653

n = 6

Au	-2.596949	-2.077120	-0.002244
Au	0.000607	-0.005087	2.167618
Au	-2.592169	2.081447	0.001145

Au	-0.000519	0.002216	-2.164385
Au	2.595849	2.078349	0.001062
Au	2.593181	-2.079867	-0.003121
Li	-2.454355	0.001101	1.429546
Li	-0.001399	-1.576347	-0.001891
Li	0.001288	1.575047	0.003741
Li	-2.457029	0.002957	-1.431041
Li	2.456032	0.000869	-1.431748
Li	2.455454	-0.001993	1.429432

$n = 7$

Au	2.549721	-1.245154	2.018020
Au	-0.005589	-2.622908	-1.554775
Au	0.000208	-0.047422	-0.207319
Au	0.006834	3.125788	1.511829
Au	2.126675	1.006842	-1.884535
Au	-2.557767	-1.232978	2.015865
Au	-2.120092	1.016988	-1.886509
Li	-0.004991	-1.673517	1.759842
Li	1.657763	1.113502	1.350575
Li	2.178075	-1.364785	-0.519679
Li	0.006078	2.425997	-0.949828
Li	0.000505	-0.298762	-2.800010
Li	-2.183939	-1.354004	-0.521450
Li	-1.653215	1.121137	1.349369

$n = 8$

Au	-1.811158	2.980450	1.255491
Au	-3.270377	-0.714519	0.039311
Au	-0.592553	1.348506	-2.664771
Au	-0.255978	-0.238545	-0.090487
Au	2.736941	2.270072	-0.025607
Au	-0.383909	-3.190985	-1.233659
Au	0.134215	-1.459249	2.716790
Au	3.502222	-0.976838	-0.002092
Li	-2.339616	1.559023	-0.761255
Li	-1.570119	0.527383	1.982196
Li	0.255884	2.474631	-0.207592
Li	-1.492931	-2.400388	0.910946
Li	-1.579671	-1.060384	-2.120829
Li	1.436089	-2.308230	0.391416
Li	1.867420	0.358177	-1.506937
Li	1.858658	0.352301	1.444368

$n = 9$

Au	-2.959850	-2.093656	-0.265666
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Au	-0.458906	2.168624	-1.911217
Au	-2.959879	2.093911	-0.263193
Au	-0.458956	-2.166208	-1.914033
Au	0.745798	0.000498	-0.176845
Au	-1.473251	-0.001954	2.921879
Au	3.260141	0.001192	-1.835578
Au	2.112539	2.218261	1.714588
Au	2.112706	-2.220653	1.712041
Li	-1.831184	0.000734	-1.259662
Li	-0.740980	1.802268	0.997193
Li	-3.395571	-0.000793	1.136761
Li	0.752408	0.001705	-2.831870
Li	-0.740631	-1.803426	0.994557
Li	1.920244	2.206353	-0.932946
Li	1.919860	-2.204770	-0.935315
Li	1.007662	-0.001781	2.510585
Li	3.205831	-0.000681	0.795358

(2) The cartesian coordinates of (AuLi)<sub>n</sub>-CO (*n* = 1-9) clusters

Bridge adsorptions

*n* = 1

Au	0.445820	-0.054050	0.000008
Li	-0.707824	1.973729	-0.005168
C	-1.971707	0.414003	0.006860
O	-2.658263	-0.516905	-0.003287

*n* = 2

Au	1.833816	-0.486330	-0.000063
Au	-2.250547	0.079139	0.000090
Li	-0.046791	1.216406	-0.001698
Li	-0.420080	-1.537748	0.001274
C	1.841333	2.127504	-0.004524
O	2.909288	2.545891	0.003283

*n* = 3

Au	-0.336487	-1.545600	0.001991
Au	-2.106753	0.971486	-0.001001
Au	2.099961	1.264846	-0.000073
Li	2.131295	-1.270821	0.002482
Li	-0.047516	0.667295	-1.334512
Li	-0.048406	0.670575	1.334243
C	1.696213	-3.283141	-0.003406
O	1.354455	-4.383763	-0.007327

$n = 4$

Au	0.093055	2.043790	1.405182
Au	-2.459145	-0.002089	-1.030016
Au	1.550094	-0.004784	-1.792561
Au	0.092543	-2.037059	1.415097
Li	1.558728	0.001638	0.818685
Li	-0.392762	1.500417	-1.036070
Li	-0.393490	-1.505470	-1.028791
Li	-1.442932	0.003383	1.322850
C	3.626255	0.001069	0.250468
O	4.675828	0.000605	-0.193910

$n = 5$

Au	2.087579	1.954747	-0.234687
Au	-1.681972	1.779384	-1.185683
Au	-0.523831	0.012852	2.104809
Au	2.248480	-1.784067	-0.162401
Au	-1.507745	-1.978376	-1.115016
Li	2.069681	0.113603	1.430731
Li	-0.170743	2.283162	0.720628
Li	0.342966	-0.011721	-1.043336
Li	-2.471583	-0.115395	0.255100
Li	0.028100	-2.268356	0.816389
C	-3.238190	0.040046	2.270741
O	-3.643073	0.122143	3.335291

$n = 6$

Au	-2.322051	-2.488332	-0.001591
Au	0.008745	0.087181	2.146661
Au	-2.783910	1.642547	0.001423
Au	0.007202	0.094241	-2.144886
Au	2.604138	2.043640	0.000855
Au	2.696734	-2.093366	-0.002807
Li	-2.405430	-0.421277	1.442965
Li	0.134401	-1.557570	-0.001787
Li	-0.044687	1.652782	0.003291
Li	-2.406298	-0.419449	-1.443275
Li	2.479487	-0.022501	-1.437394
Li	2.480346	-0.024907	1.435467
C	-0.966401	3.606475	0.002553
O	-1.446607	4.644103	0.001784

$n = 7$

Au	-1.816284	-2.481631	1.760964
Au	-2.406844	-0.023669	-1.870459
Au	0.008372	-0.008164	-0.209328

Au	2.609400	0.029066	2.160459
Au	1.224928	-2.156409	-1.731554
Au	-1.773058	2.584827	1.647337
Au	1.260598	2.058299	-1.812576
Li	-2.164861	0.042627	1.168054
Li	0.611121	-1.590408	1.692699
Li	-1.265105	-2.206112	-0.727464
Li	2.555645	-0.038253	-0.505475
Li	0.082397	-0.061002	-2.826523
Li	-1.232250	2.186944	-0.825373
Li	0.642784	1.659790	1.607235
C	4.601372	-0.019997	0.150698
O	5.655090	-0.005492	0.587981

$n = 8$

Au	2.445707	-2.103728	1.726298
Au	2.733150	1.783946	0.324964
Au	1.178436	-1.174824	-2.408085
Au	0.056606	0.322614	-0.042922
Au	-1.908393	-3.028207	0.003237
Au	-0.622957	3.145427	-1.421013
Au	-0.973857	1.492155	2.591215
Au	-3.729578	-0.180606	-0.363609
Li	2.827794	-0.731676	-0.392402
Li	1.353830	0.166943	2.177924
Li	0.502423	-2.374631	0.058297
Li	0.430128	2.838725	0.864477
Li	1.261283	1.456608	-1.985105
Li	-2.222476	1.753810	0.074092
Li	-1.593079	-1.022636	-1.572198
Li	-1.925567	-0.832510	1.338765
C	4.153657	-1.469821	-1.940063
O	4.753133	-1.903811	-2.805985

$n = 9$

Au	2.911221	-0.919228	-2.031857
Au	0.191597	-1.679857	2.342826
Au	2.939553	-0.536300	2.127636
Au	0.161786	-2.080929	-1.990799
Au	-0.703127	0.012396	0.009339
Au	2.070676	2.719831	-0.254379
Au	-3.474253	-1.129117	0.120499
Au	-1.702472	2.349061	2.028579
Au	-1.716232	1.951694	-2.391960
Li	1.619303	-1.476013	0.125855
Li	0.999173	1.086502	1.681227

Li	3.607904	0.588412	-0.078041
Li	-1.209615	-2.651624	0.264632
Li	0.976718	0.764108	-1.854862
Li	-1.958999	-0.259765	2.274900
Li	-1.976253	-0.657644	-2.161267
Li	-0.448438	2.690301	-0.235829
Li	-2.932917	1.453413	-0.113443
C	-3.003857	-3.847537	0.251183
O	-3.953577	-4.480553	0.244066

### Top adsorptions

$n = 1$

Au	-0.323828	-0.079362	-0.000004
Li	-2.222650	1.381214	0.000048
C	1.820435	-0.297997	0.000069
O	2.665965	0.489246	-0.000026

$n = 2$

Au	1.774122	-0.313842	0.000448
Au	-2.459915	0.118217	-0.000161
Li	-0.396731	-0.117825	1.315362
Li	-0.397773	-0.129649	-1.315019
C	3.854640	0.525753	-0.000726
O	4.179168	1.630283	-0.002424

$n = 3$

Au	-2.425318	-1.074090	0.000305
Au	1.896443	-0.467113	-0.003529
Au	-0.079990	1.861317	0.001331
Li	-2.482680	1.435600	0.002630
Li	-0.295895	-0.348740	1.304333
Li	-0.301398	-0.346021	-1.304888
C	3.899222	-1.334381	0.007272
O	4.243106	-2.438163	0.012463

$n = 4$

Au	0.780620	1.346026	-2.026401
Au	0.750477	1.337956	2.038732
Au	-2.309588	-0.630287	-0.018958
Au	1.612107	-2.079937	0.006333
Li	-0.136225	-0.970575	-1.481525
Li	-0.775297	1.474339	-0.004938

Li	-0.158538	-0.976599	1.472304
Li	2.039141	0.446080	0.013787
C	-4.566793	-0.405119	-0.012695
O	-5.170269	0.573012	0.012568

$n = 5$

Au	-2.146045	-1.895540	-0.222760
Au	1.605482	-1.885906	-1.136054
Au	0.428856	0.000193	2.135401
Au	-2.146862	1.895333	-0.222923
Au	1.605738	1.885665	-1.136624
Li	-2.129282	-0.000006	1.379702
Li	0.087643	-2.292745	0.783366
Li	-0.341137	0.000021	-1.009306
Li	2.413473	-0.000107	0.293795
Li	0.087381	2.292787	0.782181
C	3.408048	0.001037	2.211564
O	3.846385	0.001761	3.261908

$n = 6$

Au	2.308514	-2.089397	0.351672
Au	-0.156491	-1.137656	-1.252973
Au	2.710802	1.850952	-0.871674
Au	0.294347	1.001181	2.244298
Au	-2.311895	2.320194	-0.544348
Au	-2.517477	-1.663833	0.687923
Li	2.251939	-0.483962	-1.677747
Li	-0.003362	-1.413824	1.321114
Li	0.148791	1.441370	-0.440883
Li	2.542722	0.303251	1.126954
Li	-2.171276	0.730533	1.408448
Li	-2.493184	-0.062990	-1.408799
C	-2.056549	-1.293461	-3.044872
O	-1.797974	-2.002019	-3.911870

$n = 7$

Au	0.417977	-2.194967	2.694794
Au	0.012207	-2.350571	-1.979330
Au	0.108385	-0.066880	-0.192867
Au	-0.097108	2.817639	1.983482
Au	2.917294	0.229165	-0.359118
Au	-3.647809	-0.325828	0.228277
Au	-0.657270	1.800106	-2.283690
Li	-1.562433	-1.549408	1.135673
Li	0.698789	0.360605	2.244444
Li	1.409519	-2.164814	0.327519



Li	1.042536	2.317430	-0.249734
Li	1.249711	-0.074352	-2.495462
Li	-1.976118	-0.529106	-1.700386
Li	-1.829626	1.524797	0.502759
C	5.075564	0.307419	-0.066187
O	5.901129	0.714452	-0.766205

$n = 8$

Au	-0.848428	3.001405	1.271409
Au	-3.231045	0.212431	0.035288
Au	0.054011	1.480795	-2.720756
Au	-0.258200	0.191630	0.125504
Au	3.430910	1.554761	0.012955
Au	-1.179822	-3.261206	-1.257941
Au	-0.129943	-1.481401	2.647745
Au	3.218826	-1.783050	-0.045279
Li	-1.718042	2.134581	-0.954730
Li	-1.589918	0.682825	2.241826
Li	1.151448	2.488297	-0.317931
Li	-1.896947	-1.928814	0.776980
Li	-1.204972	-0.819077	-2.015556
Li	0.806591	-2.396790	0.154321
Li	1.987279	-0.002991	-1.411691
Li	2.036419	-0.068209	1.464983
C	-5.306504	0.701336	-0.619516
O	-6.290605	0.276094	-0.192818

$n = 9$

Au	-2.689147	-2.210747	-1.120729
Au	-0.797271	2.622198	-0.681376
Au	-3.144758	1.485859	0.793233
Au	-0.325737	-1.204302	-2.662872
Au	0.762745	0.083886	-0.148981
Au	-1.204501	-1.605500	2.644259
Au	3.130739	1.161443	-1.667136
Au	2.017790	1.368865	2.522659
Au	2.500888	-2.549634	0.493881
Li	-1.872772	0.234481	-1.068057
Li	-0.819169	0.951006	1.743345
Li	-3.243795	-1.051815	1.089694
Li	0.570314	1.282361	-2.510301
Li	-0.426584	-2.231676	0.094877
Li	1.630186	2.526325	0.165414
Li	2.109726	-1.367787	-1.850509
Li	1.223841	-1.094968	2.236088
Li	3.274157	-0.033013	0.673266

C	-1.630087	4.202682	-1.002420
O	-2.170777	5.515728	-1.171135